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Optimization of interdigital micromixers via analytical modeling—exemplified with the SuperFocus mixer

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Abstract

It is shown how interdigital micromixers can be optimized in a creeping laminar flow regime. This task is accomplished with an analytical model derived in this paper that does not only include the mixing channel, but also the focusing section typical for interdigital micromixers. The SuperFocus mixer, the genotype interdigital micromixers, is used for this optimization process and it is shown where its bottlenecks with respect to residence time and pressure drop lie and how these can be overcome via a design variation.

Keywords: SuperFocus; Interdigital micromixer; Optimization process

1. Introduction

Micromixers using an interdigital flow configuration are ideally suited for mixing at high volume flows [1–3]. Concerning liquid mixing, achieving short mixing times in the millisecond range was limited for most cases by a too high thickness of the fluid lamellae, typically being not smaller than a few 10 μm until the introduction of the SuperFocus mixer [4,5]. For that reason, we have chosen this mixer to show how to optimize the performance of such a microfluidic device. The most straightforward approach would be the direct simulation of the mixing process via computational fluid dynamics (CFD), since this in principle allows describing the dynamics with a high accuracy. However, it turns out that most such attempts are unmanageable on standard workstations if the result should not be distorted by discretization errors, i.e. numerical diffusion. Hence we have chosen an analytical approach. In the first section, we present the basic design and the assumptions for the calculation. After this we describe the model and some exemplary results.

2. Basic design and assumptions

The design investigated is derived from the SuperFocus mixer [4]. This design displayed in Fig. 1 was chosen since it is generic for micromixers relying on the principle of interdigital multilamination and hydrodynamic focusing.

The fluid enters through inlets equally distributed over the entrance section having a pitch dp. The entrance section spans an arc of angle α with a radius r and has a height h. We restrict ourselves to the case where the height is always the same throughout the mixer. With the techniques outlined in this abstract it can be shown that lifting this restriction allows to find mixers with an even better performance. The fluid entering through the inlets is then focused in the delta shaped region discharging into a straight channel of width w and length l. In the next section we show how such a design can be optimized. The fluidic system we use for the optimization is characterized by a constant density ρ of 10^3 kg/m^3, a dynamic viscosity η of 10^{-3} Pa s and a diffusion constant D of 10^{-9} m^2/s. These properties are typical for watery systems in which small molecules should be mixed. We assume equal volume flows for both fluids and a total volume flow $\dot{V}$ of 8 l/h.

3. Computational method

The most relevant characteristics of a mixer for a given volume flow are its pressure drop, mean residence time, and mean mixing quality. In principle, these numbers are accessible through the use of modern CFD tools utilizing a finite-volume- or finite-element-method. However, as shown by Hardt and Schönfeld [6] when studying liquid mixing processes, artifacts due to numerical diffusion are likely to dominate the simulation results on diffusive mixing typical for interdigital micromixers. Therefore, we have chosen a

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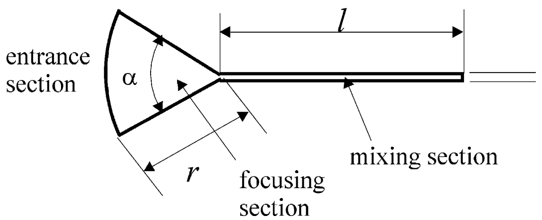

Fig. 1. SuperFocus design.

different approach, semi-analytical approach to quantify the SuperFocus mixer.

Previous CFD simulations [6] have indicated that in triangular focusing mixers with an acute-angled focusing section nearly no lamella tilting in the mixing channel can be observed. The agreement of the simulations and experiments was also verified by the same authors. This behavior is typical for the creeping laminar regime [7]. Furthermore we assume that the lamellae are uniformly distributed. This is true if we have a pure plug flow and all lamellae have the same volume flow. Deviations from this assumption will be discussed further below. Under these circumstances the time independent convection–diffusion problem can be mapped on a time dependent diffusion problem. We have to change from the lab-to a co-moving reference frame.

In this frame, each lamella initially has a width of $\mathrm{d}p$. This width is then reduced to $\mathrm{d}p\, w/\alpha r$ in the focusing channel. Neglecting the outermost lamella we have a diffusion problem with a location varying length scale. This location is indicated by the variable y in the following. As the relevant length scale we chose the width of a lamella $wf(y)$. Thus, the diffusion equation changes from

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2} \tag{1}$$

to

$$\frac{1}{\pi^2}\frac{\partial c}{\partial \beta(y)} = \frac{\partial^2 c}{\partial \zeta(y)^2} \tag{2}$$

where we define a dimensionless time $\partial\beta(y) = D^2\pi^2/(wf(y)^2)\partial t$ and dimensionless space coordinate $\partial\zeta(y) = 1/(wf(y))\partial x$. Since these variables change with location it does make only sense to introduce them in a differential way, because their absolute value is defined by the history of the streamline. At this point it should be also pointed out that the value range for the dimensionless variables is the same for all locations, namely from zero to infinity for the time and minus one to one for location. In the non-transformed reference frame, this would not have been true since the width of the lamella is different for different locations. The solution of the dimensionless differential diffusion equation is then [8]

$$c(\beta,\zeta) = \frac{1}{2} + \sum_{n=1,3,\ldots} \frac{2(-1)^{(n-1)/2}}{n\pi}\,\mathrm{e}^{-n^2\beta}\cos(n\pi\zeta) \tag{3}$$

where initial concentrations of 0 and 1 have been assigned to the different liquids. From this formula the value of β can be determined at which a certain mixing quality ε is achieved, according to

$$\varepsilon = 1 - \sqrt{\frac{1}{2}\int_{-1}^{1}\left|c(\beta,\zeta)-\frac{1}{2}\right|^2 \mathrm{d}(\zeta)} \tag{4}$$

For a mixing quality of 0.99 the corresponding β would be 4.5. Thus, for a given focusing section one only needs to determine how long the mixing channel needs to be to yield the relevant β value. The main advantage of this description is that it allows determining the mixing in the delta shaped focusing region.

Since the fluid is incompressible, the velocity u is given by

$$u = \frac{\dot{V}}{A} \tag{5}$$

where A is the channel cross-section. For the focusing section $A = \alpha r' h$, where r' is the local radius, while for the mixing channel the cross-section is given by wh. The corresponding lamella widths are then $(r'/r)\mathrm{d}p$ and $(\mathrm{d}p/r)w$. Combining these formulae the dimensionless mixing time for the full mixer is given by

$$\begin{aligned}\beta &= D\pi^2 \\ &\quad\times\left[\int_r^{w/2}\left(\frac{r}{\mathrm{d}p\, r'}\right)^2\frac{\alpha r' h}{\dot{V}}\,\mathrm{d}r' + \int_0^1\left(\frac{\alpha r}{\mathrm{d}p\, w}\right)^2\frac{wh}{\dot{V}}\,\mathrm{d}x'\right] \\ &= D\pi^2\frac{hr^2\alpha}{\mathrm{d}p\,\dot{V}w}\left(l\alpha + w\ln\left(\frac{r}{w/2}\right)\right)\end{aligned} \tag{6}$$

analogously the residence time T is given by

$$T = \int_r^{w/2}\frac{\alpha r' h}{\dot{V}}\,\mathrm{d}r' + \int_0^l\frac{wh}{\dot{V}}\,\mathrm{d}x' \tag{7}$$

The last quantity missing is the pressure drop. For the calculation of the pressure drop in the mixing channel we utilized the formula offered by Knight et al. [9]

$$\Delta p_\mathrm{m} = 2\eta\left(4.7 + 19.64\frac{1+(w/h)^2}{(1+w/h)^2}\right)\left(\frac{h+w}{2hw}\right)^2\frac{l\dot{V}}{hw} \tag{8}$$

This is not the most precise approximation that can be found in the literature. However, it is symmetric with respect to the aspect ratio of the channel and therefore ideal for a semi-analytical optimization. Since there is no closed general formula available for the pressure drop in the focusing section we have taken Eq. (8) and integrated it over r, yielding

$$\begin{aligned}\Delta p_\mathrm{e} &= \frac{\eta\dot{V}}{\alpha h}\left(\frac{6.085}{\alpha^2}\left(\left(\frac{w}{2}\right)^{-2} - r^{-2}\right)\right. \\ &\quad\left. + \frac{4.7}{\alpha h}\left(\left(\frac{w}{2}\right)^{-1} - r^{-1}\right) + \frac{12.17}{h^2}\ln\left(\frac{ra}{w/2}\right)\right)\end{aligned} \tag{9}$$

At this point approximate analytical formulae for all relevant properties are available. Before we use these formulae

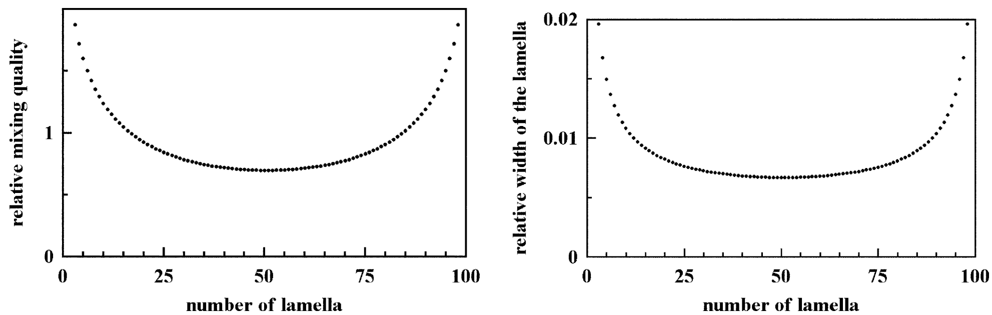

Fig. 2. Relative width (right) in a parallel plate channel with 100 lamellae and corresponding relative mixing quality (left).

for the design optimization we want to outline one of the limits of our model. The major assumption is the plug flow in the mixer. To get an idea which deviations in an experiment from out model can be expected we investigate a non-plug flow situation. To be able to use analytical methods we look at the flow between parallel plates, since for this situation the velocity field is analytically know, namely for parallel plates the velocity profile is given by

$$u(x) = \frac{3\bar{u}}{2}\left[1 - \left(\frac{2x}{w}\right)^2\right] \tag{10}$$

where $\bar{u}$ is the mean velocity and w the distance separating the plates. Since we assumed that each lamella corresponds to the same volume flow the width of the lamellae, in case they are parallel to the plates, varies over the width of the channel as can be seen in Fig. 2 on the right hand side. Using the dimensionless time β one can also derive the relative mixing quality as shown in Fig. 2 on the left hand side. Here the relative mixing quality is the mixing quality ($\propto \exp(-\beta)$) of a lamella after a certain length of the channel divided by the mean mixing quality over all lamella after the same channel length.

As expected, these results show that in reality one does not obtain a single number for the mixing quality but a mixing quality distribution. As can be seen on the left hand side of Fig. 2, the mixing quality of the outer lamellae is worse than in the middle as the width of these lamellae is larger. However, there is only a factor of 3.79 between the minimum and the maximum mixing quality. This value is not higher since the wider lamellae also move slower.

4. Results

In the following, we investigate how to optimize the SuperFocus design and show which impact each design parameter has. The most straight forward parameter is the pitch dp, since a reduction of dp reduces the time needed to achieve a certain mixing quality, i.e. β is increased and hence the critical β is reached earlier, while having no impact on any other characteristics in the framework of our model. Thus, in a realistic situation this parameter will be determined by factors like manufacturability and mechanical stability and, therefore, we fix it in our investigation to a value of 0.1 mm. The parameter to consider is the angle of the focusing section. An increase of this value raises the number of lamellae. However, it increases also the residence time. In the case where one keeps the product of angle and radius fixed, i.e. the radius is reduced when the angle is increased, the mixing quality and the pressure drop in the mixing channel stays constant while the pressure drop and the residence time in the focus are reduced. Accordingly, an increase of the opening angle coincides with an improvement of the mixer. However, one has to be aware that for too large opening angles the tiling of the lamellae at the transition from the focusing to the mixing section get more likely and, therefore, the performance of the mixer can no longer be evaluated with our model. Hence we fix the angle to a value of 50° in our further calculations.

After having fixed the more trivial design parameters, there are still four open parameters, namely the radius r, the height h, the length of the mixing channel l, and the width of the mixing channel w. As mentioned above we always aim for a mixing quality of 99%. Since in most cases one has a maximum allowed pressure drop we do our investigations with a set of different, but fixed pressure drops. In the same sense, we proceed with the height of the mixers, where about 50 different values for h were considered. Usually, the maximum height is limited due to manufacturing reasons, which is the reason why we proceed in the described manner. Correspondingly, the height and the pressure drop are, strictly speaking, no variation parameters, and only the width of the mixing channel is a parameter that is used for the identification of the optimum.

As can be seen from Fig. 3, the residence time can be reduced via an increase of the pressure drop. However, our model shows that there is no linear dependence, but a power law with the exponent −0.775. The second conclusion that can be drawn from Fig. 3 is that there is a limiting asymptotic minimum residence time reached for large heights.

The corresponding geometric parameters are displayed in Fig. 4. The radius of the focusing section and the width of the mixing channel are monotonically decreasing functions of the height. Also, both parameters are decreasing with increasing pressure. However, the length of the mixing channel

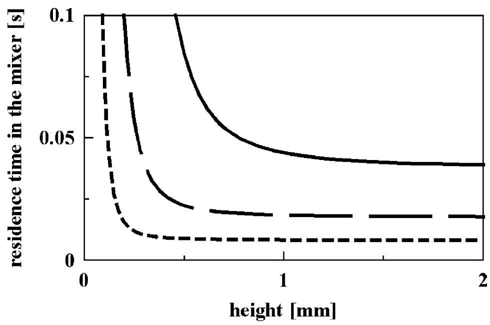

Fig. 3. Residence time for three different pressure drops (full line: 0.1 bar, dashed line: 1.0 bar, short dashed line: 10 bar) and a final mixing quality of 99%.

has an inverse behavior with respect to pressure and shows a maximum for a certain height. Interestingly, the length of the mixing channels seems to reach a common value for all pressure drops for large heights.

A key question we are able to answer with the given model is how much of the mixing actually takes place in the focusing section. This is a point formerly neglected in the analysis of this type of mixer. From Fig. 5 we can see that the mixing in the focusing region is reduced via increasing pressure drop and height. However, we also have to realize that the relative residence time in the focusing section does not fall below a value of about 67%. Thus, the focusing region is the main bottleneck with respect to the residence time. With respect to the pressure drop, however, the situation is reversed, as can be seen in Fig. 5. Therefore, the aim for the optimization is to overcome these two bottlenecks in one go. One solution is to lift the initial set condition of a common height for the whole of the mixer. The reason for this is quite trivial, namely a reduction of the height in the focusing section reduces the residence time and an increase in the height in the mixing channel reduces the pressure drop. One could now modify the model to incorporate this height variation and do the same optimization as outlined above. However, one has to be aware that in this case the optimum would have a large height variation. Hence there will be a section that has to accomplish this height variation without destroying the order of the lamellae. Therefore, it would be crucial to identify designs via CFD that fulfill this task and then to integrate a good model for these.

Finally, we should mention that the CPU time needed for these calculations was less than 1 min. Thus, such an approach is ideal for system optimization.

5. Outlook and conclusions

We have shown at the example of the SuperFocus interdigital micromixer that analytical methods can be powerful for optimization of microfluidic systems and how one can address even issues that are out of reach for CFD calculations up to now. We also showed how to identify bottlenecks of this mixer and proposed a new class of SuperFocus mixers that should have an improved performance. The

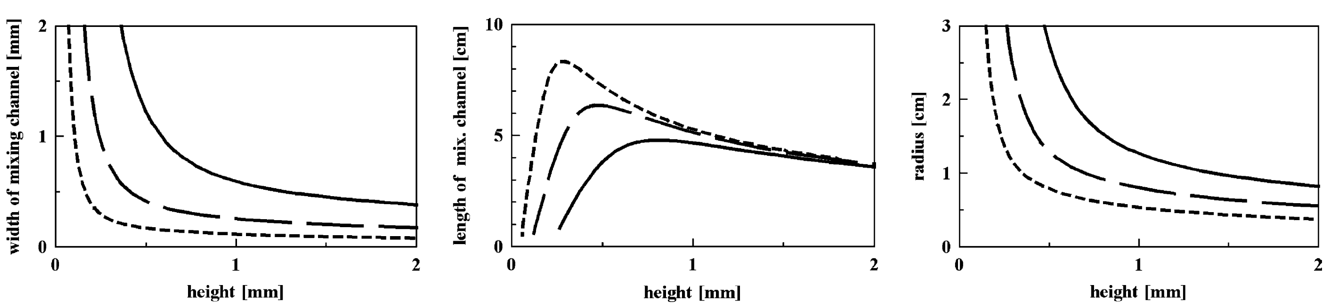

Fig. 4. Width (left) and length (middle) of mixing channel and radius of the entrance section (right) for three different pressure drops (full line: 0.1 bar, dashed line: 1.0 bar, short dashed line: 10 bar) and a final mixing quality of 99%.

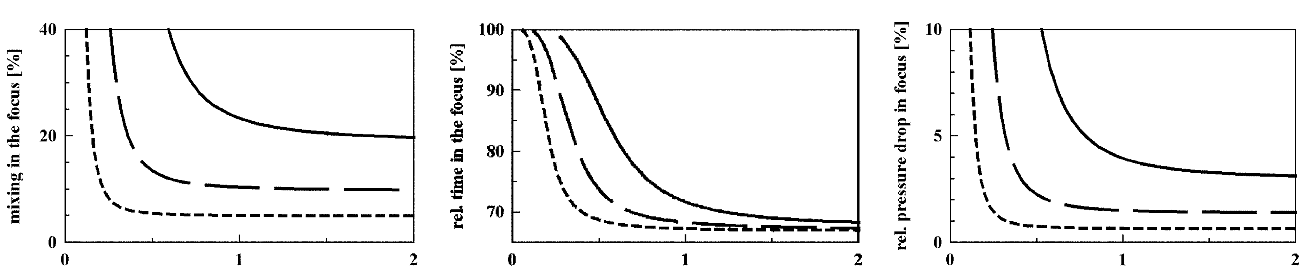

Fig. 5. Percentage of the mixing (left) and residence time (middle) and pressure drop (right) in the focusing section for three different pressure drops (full line: 0.1 bar, dashed line: 1.0 bar, short dashed line: 10 bar) and a final mixing quality of 99%.

calculations presented here can easily be extended to incorporate also mechanical aspects as the deformation of the inlet walls separating the fluid streams in the entrance region or thermal aspects when chemical reactions are involved.

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